Supporting Information

for ***Physical Chemistry Chemical Physics***

Supporting Information

Effect of Meta Coupling on Colour Purity, Quantum Yield, and Excitons Utilizing Efficiency in Deep-Blue Emitters from Phenanthroimidazole Isomers

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1. S3 to S5 and T3 to T5 NTOs of BPPI, L-BPPI and Z-BPPI (Fig.S1 to Fig.S3)

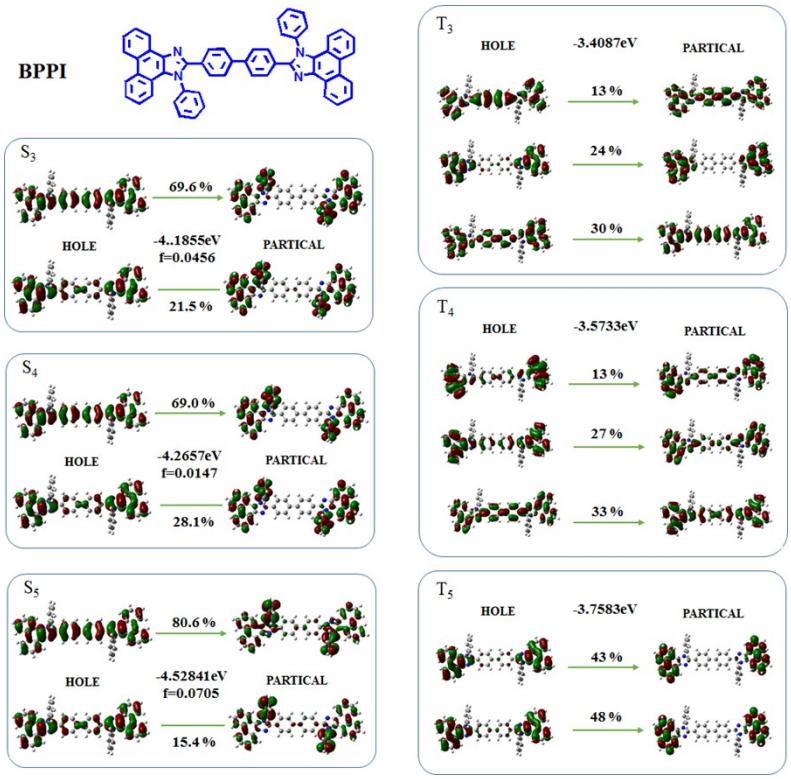

Fig. S1 S3 to S5 and T3 to T5 NTOs of BPPI

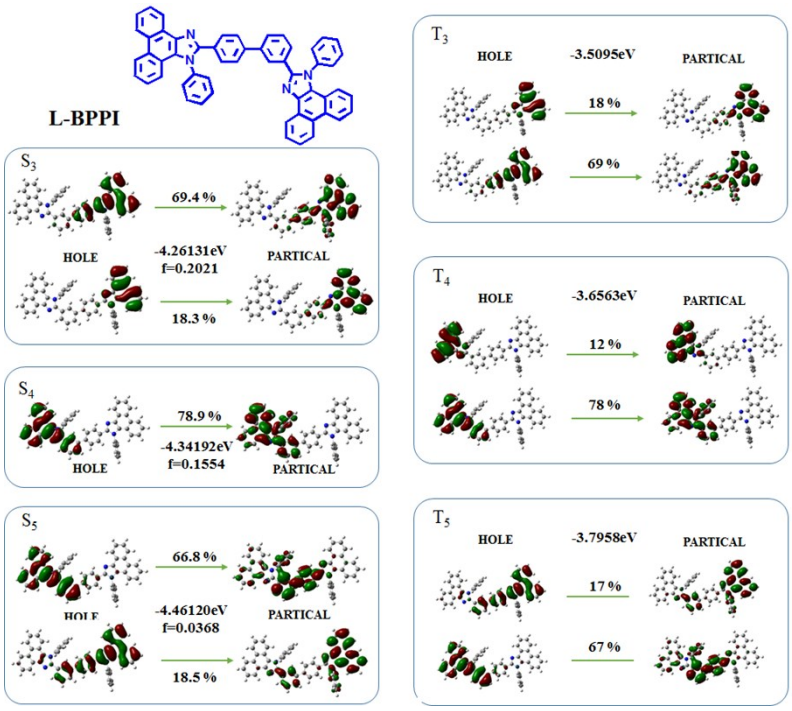

Fig. S2 S3 to S5 and T3 to T5 NTOs of L-BPPI

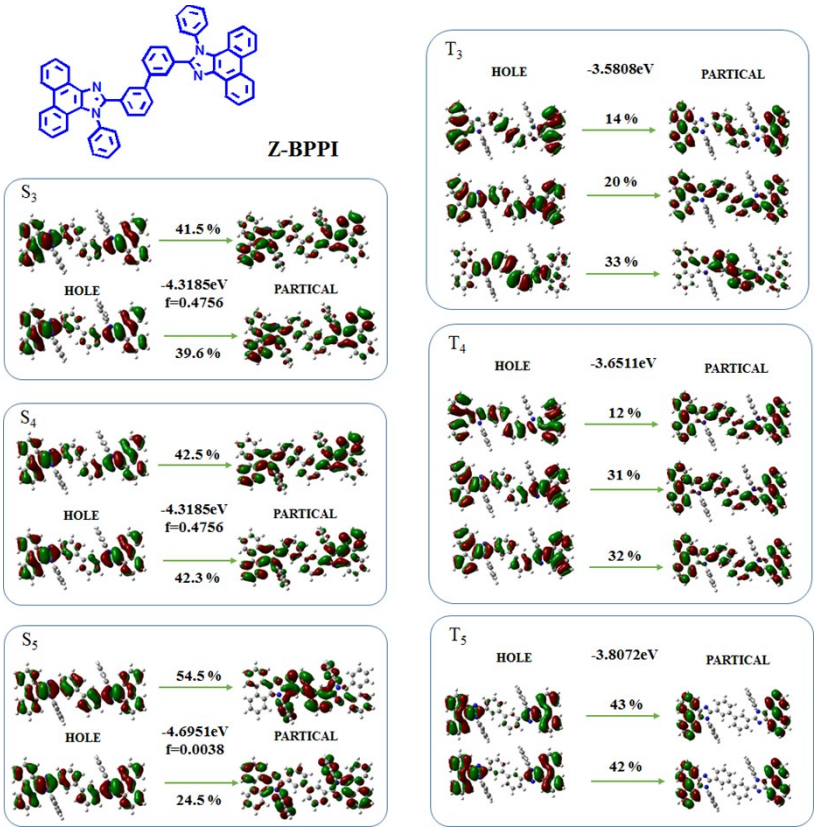

Fig. S3 S3 to S5 and T3 to T5 NTOs of Z-BPPI

2. The solvatochromic Lippert-Mataga model

The Lippert-Mataga model is estimated according to **Equation 1** as shown below:

$$hc(\nu_a - \nu_f) = hc(\nu_a^0 - \nu_f^0) + \frac{2(\mu_e - \mu_g)2}{a_0^3} f(\varepsilon,n) \qquad \textbf{Equation S1}$$

where h is the Plank constant, c is the light speed in vacuum, $f(\varepsilon,n)$ is the orientational polarizability of solvents and $f(\varepsilon,n) = \left[\frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 - 1}\right]$, $\nu_a^0 - \nu_f^0$ is the Stokes shifts when f is zero, a_0 is the solvent Onsager cavity radius, μ_e and μ_g are dipole moments of excited-state and ground-state, respectively. ε is the solvent dielectric constant and n is the solvent refractive index. a_0 and μ_g were estimated at the level of b3lyp/6-31g(d,p) from the Gaussian09 package.

Table-S1 The solvatochromic properties of BPPI (a_0=0.714 nm and μ_g = 4.579D)

	BPPI			
Solvents	$f(\varepsilon,n)$	λ_a (nm)	λ_f (nm)	$\nu_a - \nu_f$ (cm^{-1})
Hexane	0.0012	368	412	2902.06838
Ethylamine	0.048	369	414	2945.68163
Butylether	0.096	370	415	2930.64148

Ethylether	0.167	368	415	3077.52750
Ethylacetate	0.2	368	419	3307.56459
Tetrahydrofuran	0.21	369	421	3347.30188
Acetone	0.284	366	443	4749.04094
Acetonitrile	0.305	365	445	4925.35016

Results: In low-polarity solvents (the former six):

Slope = 2093.37370337; Correlation = 0.90452685; $\mu_e =$ 7.80178524

In high-polarity solvents (the latter five):

Slope = 14721.10104476; Correlation = 0.98619292; $\mu_e =$ 20.68905984

Table-S2 The solvatochromic properties of L-BPPI (a_0=0.714 nm and $\mu_g =$ 3.872D)

L-BPPI				
Solvents	$f(\varepsilon,n)$	λ_a (nm)	λ_f (nm)	$\nu_a - \nu_f$ (cm^{-1})
Hexane	0.0012	363	383	1438.54879
Ethylamine	0.048	364	386	1565.79172
Butylether	0.096	363	387	1708.41608
Ethylether	0.167	363	389	1841.26849
Ethylacetate	0.2	362	399	2561.65275
Tetrahydrofuran	0.21	363	401	2610.55351
Acetone	0.284	362	415	3527.92385
Acetonitrile	0.305	361	419	3834.48258

Results: In low-polarity solvents (the former four):

Slope = 2052.42426590; Correlation =0.95236987; $\mu_e =$ 7.72510123

In high-polarity solvents (the latter five):

Slope = 13506.70852927; Correlation =0.99168509; $\mu_e =$ 19.81734057

Table-S3 The solvatochromic properties of Z-BPPI (a_0=0.714 nm and $\mu_g =$ 2.625D)

Z-BPPI				
Solvents	$f(\varepsilon,n)$	λ_a (nm)	λ_f (nm)	$\nu_a - \nu_f$ (cm^{-1})
Hexane	0.0012	362	366	301.90502
Ethylamine	0.048	363	368	374.29632
Butylether	0.096	362	368	450.39635
Ethylether	0.167	362	369	524.03839
Ethylacetate	0.2	361	369	600.56002
Tetrahydrofuran	0.21	362	370	597.28237

Acetone	0.284	361	373	891.17955
Acetonitrile	0.305	360	371	823.59988

Results: In all solvents:

Slope =304.76060288; Correlation = 0.95532553; $\mu_e =$ 6.99263925

3. Electroluminescence devices of BPPI, L-BPPI and Z-BPPI

The relationship between EQE and EUE.

$$\eta_{EL} = \eta_{rec} \times \eta_s \times \eta_{PL} \times \eta_{out} \qquad \textbf{Equation S2}$$

Equation 2. η_{out} (~$1/2n^2$) is the light out coupling efficiency (for glass substrates, n=1.5, η_{out} is estimated as ~20%), η_{rec} is the electron-hole recombination proportion, which is assumed to be 100%, η_{PL} is the quantum yield in the solid state, and η_s is the EUE

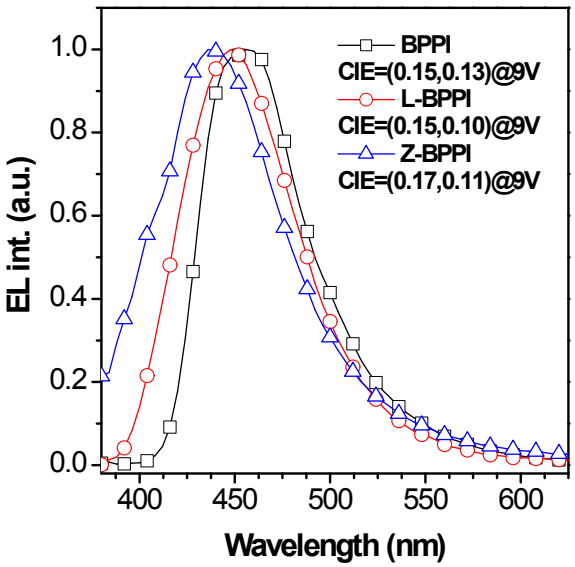

Fig. S4 The EL spectra and their CIE @ 9V

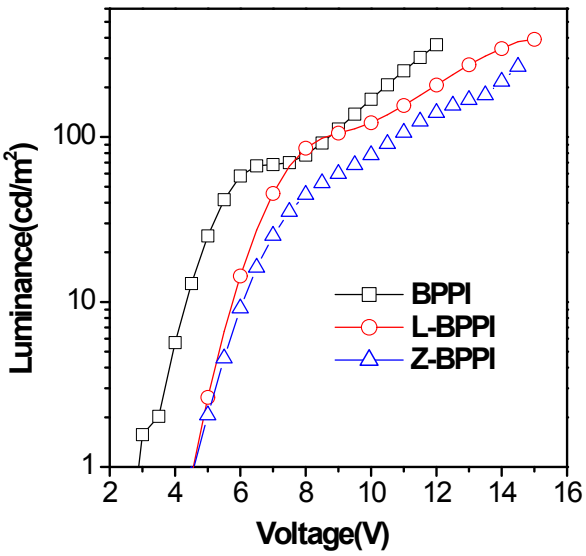

Fig. S5 The luminance versus voltage in the BPPI, L-BPPI and Z-BPPI devices

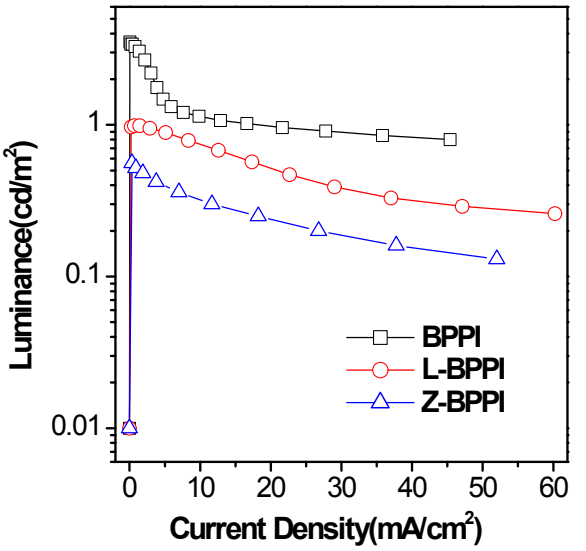

Fig. S6 The current efficiency vs current density curves in the BPPI, L-BPPI and Z-BPPI devices